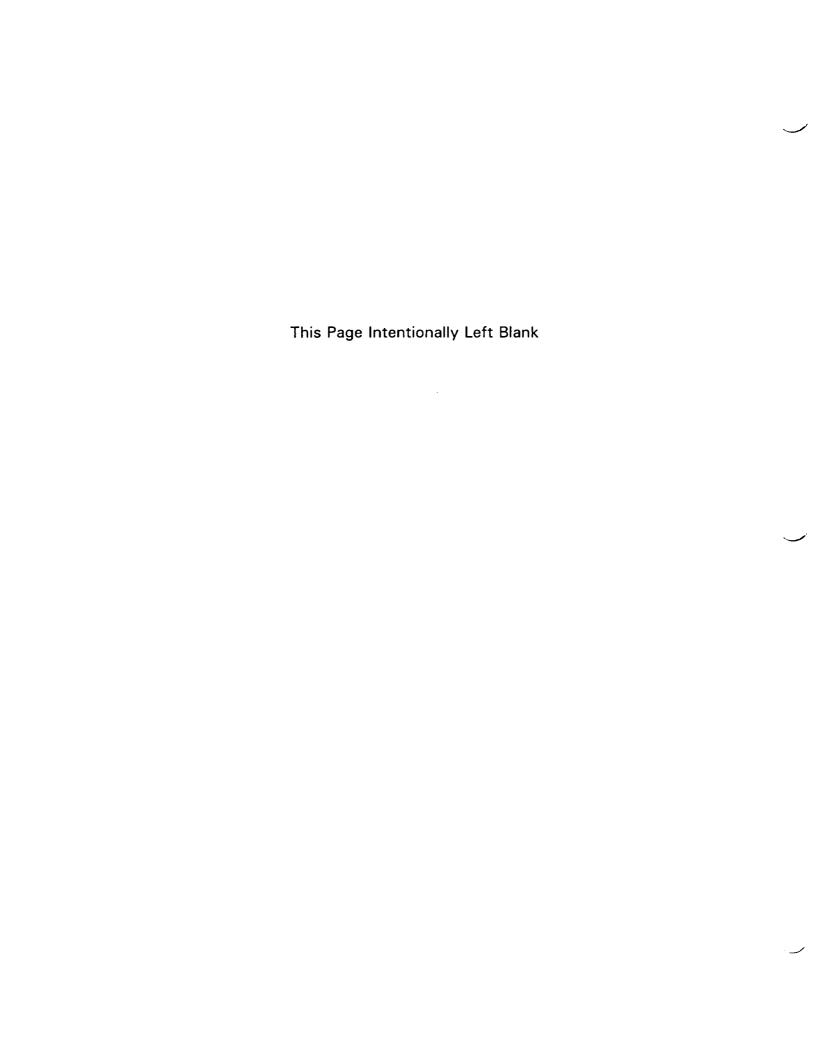
Background Document C:

Chemicals Evaluated But Not Selected as Constituents of Concern

Utah Chemical Agent Rule (UCAR)



FOREWORD

This document provides general background information on each of the chemical agents and associated chemicals that were evaluated for the proposed Utah Chemical Agent Rule (UCAR) but that the State of Utah Department of Environmental Quality, Division of Solid and Hazardous Waste (DSHW) determined should not be proposed for regulation in any capacity. For each chemical, relevant data and information are reviewed, concluding with a discussion of why the chemical was not proposed for regulation.

The first 10 chemicals presented, HN2, PD, ED, MD, DF, QL, chlorosarin, chlorosoman, CX, and DP, were included in DSHW's initial version of the proposed rule (see Preamble Section II for details). The remaining chemicals included in this background document, PS, CN, DICDI, MA, TBA, DIMP, IPA, DMDS, OXAT, and DITH, were evaluated voluntarily by the Army. The Army provided information on each chemical to DSHW, and DSHW determined that these chemicals should not be proposed for regulation in any capacity.

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CONTENTS

FOR	EWORDiii
NOT	ATION ix
1.	HN2 [Bis(2-Chloroethyl)methylamine]
2.	PD (Phenyldichloroarsine) 4
3.	ED (Ethyldichloroarsine)
4.	MD (Methyldichloroarsine)
5.	DF (Methylphosphonyl Difluoride)
6.	QL [O-Ethyl O-(2-Diisopropylaminoethyl) Methylphosphonite]
7.	Chlorosarin (Chloro-GB or O-Isopropyl Methylphosphonochloridate) 14
8.	Chlorosoman (Chloro-GD or O-Pinacolyl Methylphosphonochloridate) 16
9.	CX (Phosgene Oxime)
10.	DP (Diphosgene or Trichloromethyl Chloroformate)
11.	PS (Chloropicrin)
12.	CN (Chloroacetophenone)
13.	DICDI (N,N'-Diisopropyl Carbodiimide)
14.	MA (Methylphosphonofluoridic Acid)
15.	TBA (Tributylamine)
16.	DIMP (Diisopropyl Methylphosphonate)
17.	IPA (Isopropyl Alcohol or 2-Propanol)

CONTENTS (Cont.)

18.	DMDS (Dimethyl Disulfide)
19.	OXAT (1,4-Oxathiane)
20.	DITH (1,4-Dithiane)
REF	ERENCES
	LIST OF TABLES
1	Environmentally Relevant Properties of HN2
2	Comparison of Some Toxicities of HN2 by Different Routes of Administration in Rats and Mice
3	Environmentally Relevant Properties of PD
4	Comparison of Some Toxicities of PD by Different Routes of Administration in Rats and Mice
5	Environmentally Relevant Properties of ED
6	Environmentally Relevant Properties of MD 9
7	Environmentally Relevant Properties of DF
8	Comparison of Some Intravenous Acute Toxicities of DF in Different Mammalian Species
9	Environmentally Relevant Properties of QL
10	Environmentally Relevant Properties of Chlorosarin
11	Environmentally Relevant Properties of CX
12	Environmentally Relevant Properties of DP
13	Environmentally Relevant Properties of PS

LIST OF TABLES (Cont.)

14	Comparison of Some Acute Toxicities of PS by Different Routes of Administration in Rodent Species
15	Environmentally Relevant Properties of CN
16	Comparison of Some Acute Toxicities of CN by Different Routes of Administration in Rodent Species
17	Environmentally Relevant Properties of DIMP
18	Oral Toxicity of DIMP in Three Mammalian Species
19	Environmentally Relevant Properties of 1,4-Oxathiane
20	Environmentally Relevant Properties of 1,4-Dithiane

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NOTATION

CAIS chemical agent identification set

CAS Reg. No. Chemical Abstracts Service Registration Number

CG phosgene (carbonyl chloride)

cm² square centimeter(s)
CN chloroacetophenone
CX phosgene oxime

°C degree(s) Celsius
°F degree(s) Fahrenheit

DF methylphosphonyl difluoride
DICDI N,N'-diisopropyl carbodiimide
DIMP diisopropyl methylphosphonate

DITH 1,4-dithiane

DMDS dimethyl disulfide

DP diphosgene (trichloromethyl chloroformate)

DSHW Division of Solid and Hazardous Waste (State of Utah)

DWEL drinking water equivalent level

ED ethyldichloroarsine

EPA U.S. Environmental Protection Agency

g gram(s)

μg microgram(s)

GB sarin (O-isopropyl methylphosphonofluoridate)
GD soman (O-pinacolyl methylphosphonofluoridate)

HD sulfur mustard [bis(2-chloroethyl) sulfide]

HN2 bis(2-chloroethyl)methylamine

 ICt_{50} concentration \times time that is incapacitating to 50% of exposed

subjects

IPA isopropyl alcohol

kg kilogram(s)

K_H Henry's Law constant

 K_{oc} organic carbon partition coefficient K_{ow} octanol/water partition coefficient

L lewisite (2-chlorovinyldichloroarsine), or liter(s)

 LCt_{50} concentration \times time that is lethal to 50% of exposed subjects

LD₅₀ dose lethal to 50% of exposed subjects

m³ cubic meter(s)

MA methylphosphonofluoridic acid

MD methyldichloroarsine

mg milligram(s)
min minute(s)
mL milliliter(s)
mol mole(s)

MW molecular weight

N.O.S. not otherwise specified

NIOSH National Institute for Occupational Safety and Health

OXAT 1,4-oxathiane

PD phenyldichloroarsine

PS chloropicrin

QL O-ethyl O-(2-diisopropylaminoethyl) methylphosphonite

RCRA Resource Conservation and Recovery Act

Rfd reference dose

RMA Rocky Mountain Arsenal

s second(s)

T, t temperature
TBA tributylamine
TDG thiodiglycol

UCAR Utah Chemical Agent Rule

Background Document C: Chemicals Evaluated But Not Selected as Constituents of Concern

1. HN2 [Bis(2-Chloroethyl)methylamine] CAS Reg. No.¹ 51-75-2

(CICH₂-CH₂-)₂N-CH₃

A. Background

HN2 is one of a series of nitrogen analogs of sulfur mustard; its vesicant properties were first noted in 1935. Many such nitrogen mustards were synthesized and investigated during World War II, when the British made small quantities of HN2 on a pilot scale. Because of its marked instability, HN2 is not regarded as a chemical agent (HQ/DA,DN,AF 1990). HN2 hydrochloride ("Mustargen," by Merck Sharp and Dohme) is used in milligram amounts for the chemotherapy of Hodgkin's disease, lymphosarcomas, chronic lymphocytic leukemia, and similar conditions (Duffy 1992). HN2 is not part of the U.S. chemical agent stockpile and is not included in any chemical agent identification set (CAIS).

B. Physicochemical Properties

The storage stability of HN2 as the free base is poor, but its salts, such as the hydrochlorides, are stable (HQ/DA,DN,AF 1990). HN2 hydrolyzes slowly in water but more rapidly in the presence of alkali (HQ/DA,DN,AF 1990). Table 1 lists environmentally relevant properties of HN2.

It may be concluded that HN2 would not persist long in the environment.

C. Toxicity

The physiological effects of nitrogen mustards are similar to those of sulfur mustard (HD), but nitrogen mustards are somewhat more effective against the eyes than is HD. As with HD, nitrogen mustards cause delayed vesicancy. Table 2 shows the lethal effects of HN2 in experimental animals by different routes of administration. It appears that only acute toxicities have been determined for HN2; however, HN2 is a mutagen and suspected of being carcinogenic.

¹ CAS Reg. No. = Chemical Abstracts Service Registry Number.

TABLE 1 Environmentally Relevant Properties of HN2

Property	Data
Empirical formula	C₅H₁₁Cl₂N
Molecular weight (MW), g/mol	156.1
Density, g/mL	1.15/20°C
Melting point, °C	-65 to -60
Boiling point, °C	75/15 torr
Vapor pressure at 20°C, torr	0.29
Aqueous solubility, g/L	Sparing

Source: HQ/DA,DN,AF (1990).

TABLE 2 Comparison of Some Toxicities of HN2 by Different Routes of Administration in Rats and Mice

Route	Type of Exposure ^a	Species	Toxicity
Intravenous	I D	Rat	1,100 µg/kg
Inhalation	LD ₅₀ LC ₅₀	Mouse	1,100 μg/kg 1,500 mg/m³/30 min
Subcutaneous	LD ₅₀	Mouse	2,600 µg/kg
Intraperitoneal	LD ₅₀	Rat	1,600 µg/kg
Intraperitoneal	LD ₅₀	Mouse	2,400 µg/kg
Oral	LD ₅₀	Rat	10,000 μg/kg

^{*} LD_{50} = dose lethal to 50% of exposed subjects.

Source: Sweet (1987).

D. Discussion

HN2, like HD, is a lethal chemical, a vesicant with delayed toxic manifestations. However, it is not considered to be a chemical agent by the Army.

HN2 is currently listed by the U.S. Environmental Protection Agency (EPA) as a 40 CFR Part 261, Appendix VIII hazardous constituent; of all the chemicals specifically addressed by the proposed UCAR, only HN2 and HD have been specifically listed by EPA in Appendix VIII. Appendix VIII has been adopted by

the State of Utah as R315-50-10, Hazardous Constituents. HN2 is currently regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. HN2 content is also considered a basis for listing hazardous waste as F999 [R315-50-9(1)].

The basis for not including HN2 as a listed hazardous waste rests on three points:

- 1. There is no reason to believe that HN2 ever existed in Utah other than, perhaps, in chemotherapeutic doses (in hospitals) or in small laboratory quantities (e.g., for research purposes);
- 2. HN2 has not been stockpiled or used as munitions fill in the United States and was not included in any CAIS; and
- 3. Had HN2 been released to the environment and come in contact with moisture, it would have hydrolyzed rapidly to less toxic products.

In accordance with the criteria defined in Section VII.A of the Preamble, the Utah Department of Environmental Quality, Division of Solid and Hazardous Waste (DSHW) proposes the following:

- Remove current 40 CFR 261.33(e) P999 designation in R315-2-11(e).
- Remove current 40 CFR 261.31 F999 designation in R315-2-10(e).
- Remove from 40 CFR 261 Appendix VII basis for listing hazardous waste F999 in R315-50-9(1).

Note that because HN2 is currently listed by EPA as a 40 CFR Part 261, Appendix VIII, hazardous constituent, and considering that Appendix VIII has been adopted by the State of Utah as R315-50-10, Hazardous Constituents, HN2 will remain an Appendix VIII hazardous constituent in Utah.

2. PD (Phenyldichloroarsine) CAS Reg. No. 696-28-6

C₆H₅AsCl₂

A. Background

Introduced by the Germans in September 1917 (Prentiss 1937) and used on a limited basis in World War I, PD was classified as a blister agent but also acts as a vomiting compound (sternutator). It has no marked superiority over other vomiting compounds that were used. PD was never loaded into munitions in the United States and is not included in any CAIS. It can be considered an historic agent.

B. Physicochemical Properties

The vapor pressure of PD at temperature t (°C) may be calculated from the following formula (Sartori 1943):

$$\log p \text{ (torr)} = 9.150 - (3164/[273 + t]).$$

PD undergoes rapid hydrolysis on exposure to moisture (HQ/DA,DN,AF 1990). Thus, it does not persist in the environment as such. Table 3 lists environmentally relevant properties of PD.

C. Toxicity

PD has an immediate effect on the eyes and a delayed effect of 30 minutes to 1 hour on skin. It blisters bare skin, but wet clothing decomposes it immediately (HQ/DA,DN,AF 1990). PD equals lewisite in systemic toxicity when administered to the shaved backs of mice (Edgewood Arsenal 1974). Table 4 shows lethal effects of PD in rats and mice by different routes of administration. It appears that only acute toxicities have been determined for PD.

Specific information on the carcinogenicity of PD is lacking, but the World Health Organization is cited by Goldman and Dacre (1989) as saying, "There is no conclusive evidence that any of the organoarsenic compounds tested for carcinogenicity in laboratory animals are carcinogenic."

TABLE 3 Environmentally Relevant Properties of PD

Property	Data
Empirical formula	C ₆ H ₅ AsCl ₂
Molecular weight (MW), g/mol	222.9
Density, g/mL	1.65/25°C
Melting point, °C	-20
Boiling point, °C	252-255
Vapor pressure at 25°C, torr	0.033 (0.113/40°C)
Aqueous solubility, g/L	Slight (reacts)

Source: HQ/DA,DN,AF (1990).

TABLE 4 Comparison of Some Toxicities of PD by Different Routes of Administration in Rats and Mice

Route	Type of Exposure	Species	Toxicity
Inhalation	LC ₅₀ *	Mouse	3,300 mg/m³/10 min
Intravenous		Mouse	
	LD ₅₀		500 µg/kg
Skin	LD ₅₀	Mouse	4,000 µg/kg
Skin	LD ₅₀	Rat	16,000 µg/kg

^a LC₅₀ = concentration lethal to 50% of exposed subjects.

Source: Sweet (1987).

D. Discussion

PD is not specifically regulated by EPA under the Resource Conservation and Recovery Act (RCRA) program, although arsenicals (i.e., arsenic-containing chemical agents and associated compounds), including PD, are incorporated into 40 CFR, Part 261, Appendix VIII, under the general notation, "Arsenic Compounds, N.O.S. (not otherwise specified)." PD is not currently regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], and PD content is not treated as a basis for listing hazardous waste as F999 [R315-50-9(1)].

PD was a World War I incapacitating or lethal chemical agent of limited use, a vesicant with delayed toxic manifestations and an immediate eye irritant. It is not part of the U.S. chemical agent stockpile and is not included in any CAIS. DSHW suggested including PD specifically in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including PD specifically as a listed hazardous waste rests on two points:

- 1. No reason exists to believe that PD ever existed in Utah other than, perhaps, in small laboratory samples; and
- 2. PD has not been stockpiled or used as munitions fill in the United States, and was not included in any CAIS.

Note also that arsenic-containing waste not specifically listed as hazardous waste may be classified as hazardous waste under the EPA toxicity characteristic (incorporated under DSHW regulation R315-2-9) as D004 if it leaches arsenic at levels greater than or equal to 5 mg/L.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

3. ED (Ethyldichloroarsine) CAS Reg. No. 598-14-1

 $C_2H_5AsCI_2$

A. Background

ED was introduced by the Germans in World War I (March 1918) (Prentiss 1937) in an effort to produce a volatile agent with a short duration of effectiveness that would act more quickly than HD and last longer in its effects than PD (HQ/DA,DN,AF 1990). World War II data indicate that ED is "comparable" to lewisite (L), but inferior to it as a casualty agent (Edgewood Arsenal 1974). ED was apparently never loaded into munitions in the United States nor included in any CAIS. It may be considered an historic agent.

B. Physicochemical Properties

ED undergoes rapid hydrolysis on exposure to moisture (HQ/DA,DN,AF 1990). Thus, it does not persist in the environment as such. Table 5 lists environmentally relevant properties of ED.

C. Toxicity

ED is irritating to the respiratory tract and with sufficient exposure will produce lung injury. Prolonged contact with either liquid or vapor blisters the skin. The vapor is irritating to the eyes, and the liquid may produce severe eye injury (HQ/DA,DN,AF 1990). The rate of detoxification is rapid when exposures are to sublethal amounts (Edgewood Arsenal 1974). The inhalation LC_{50} in the mouse is 1,555 mg/m³/10 min (Sweet 1987). No multiple-dose data are available for ED.

Specific information on the carcinogenicity of ED is lacking, but the World Health Organization is cited by Goldman and Dacre (1989) as saying that "There is no conclusive evidence that any of the organoarsenic compounds tested for carcinogenicity in laboratory animals are carcinogenic."

D. Discussion

ED is not specifically regulated by EPA under the RCRA program, although arsenicals (i.e., arsenic-containing chemical agents and associated compounds), including ED, are incorporated into 40 CFR, Part 261, Appendix VIII, under the general notation, "Arsenic Compounds, N.O.S. (not otherwise

TABLE 5 Environmentally Relevant Properties of ED

Property	Data
Empirical formula	C₂H₅AsCl₂
Molecular weight (MW), g/mol	174.9
Density, g/mL	1.66/20°C
Melting point, °C	< -65
Boiling point, °C	156
Vapor pressure at 20°C, torr	2.09 (15.1/50°C)
Aqueous solubility, g/L	Slight (reacts)

Sources: HQ/DA,DN,AF (1990); Edgewood Arsenal (1974).

specified)." ED is not currently regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. Neither is ED content treated as a basis for listing hazardous waste as F999 [R315-50-9(1)].

ED was a World War I incapacitating or lethal chemical agent of limited use, a vesicant with delayed toxic manifestations, and an immediate eye irritant. It is not part of the U.S. stockpile, was never loaded into munitions in the United States, and was not included in any CAIS. DSHW suggested including ED specifically in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including ED specifically as a listed hazardous waste rests on two points:

- 1. There is no reason to believe that ED ever existed in Utah other than, perhaps, in small laboratory samples; and
- 2. ED has not been stockpiled or used as munitions fill in the United States and was not included in any CAIS.

Note also that arsenic-containing waste not specifically listed as hazardous waste may be classified as hazardous waste under the EPA toxicity characteristic (incorporated under DSHW regulation R315-2-9) as D004 if it leaches arsenic at levels greater than or equal to 5 mg/L.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

4. MD (Methyldichloroarsine) CAS Reg. No. 593-89-5

CH₃AsCl₂

A. Background

Following the use of ED by the Germans in the spring of 1918 (World War I), the U.S. Chemical Warfare Service investigated the similar, but somewhat more volatile, MD in the latter half of 1918 in an effort to produce a volatile skin and lung irritant. MD was apparently never loaded into munitions in the United States or included in any CAIS. It may be considered an historic agent.

B. Physicochemical Properties

The vapor pressure of MD at any temperature t (°C) may be calculated from the following equation (Sartori 1943):

$$\log p \text{ (torr)} = 8.6944 - 2281.7/(273 + t).$$

MD undergoes very rapid hydrolysis on exposure to moisture (HQ/DA,DN,AF 1990). Thus, it does not persist, as such, in the environment. Table 6 lists environmentally relevant properties for MD.

C. Toxicity

MD causes immediate irritation to the eyes and nose, with blistering effects delayed for hours. MD is irritating to the respiratory tract and will produce lung injury upon sufficient exposure. Prolonged contact with either liquid or vapor blisters the skin. The liquid may produce severe eye injury (HQ/DA,DN,AF 1990). The inhalation LC_{50} in the mouse is 2,700 mg/m³/10 min (Sweet 1987).

No multiple-dose data are available for MD. Specific information on the carcinogenicity of MD is lacking, but the World Health Organization is cited (Goldman and Dacre 1989) as saying, "There is no conclusive evidence that any of the organoarsenic compounds tested for carcinogenicity in laboratory animals are carcinogenic."

TABLE 6 Environmentally Relevant Properties of MD

Property	Data
Empirical formula	CH ₃ AsCl ₂
Molecular weight (MW), g/mol	160.86
Density, g/mL	1.836/20°C
Melting point, °C	-55
Boiling point, °C	133
Vapor pressure at 20°C, torr	7.76 (2.17/0°C)
Aqueous solubility, g/L	1 (with rapid hydrolysis)

Sources: HQ/DA,DN,AF (1990); Sartori (1943).

D. Discussion

MD is not specifically regulated by EPA under the RCRA program, although arsenicals (i.e., arsenic-containing chemical agents and associated compounds), including MD, are incorporated into 40 CFR, Part 261, Appendix VIII, under the general notation, "Arsenic Compounds, N.O.S. (not otherwise specified)." MD is not currently regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. MD content is not treated as a basis for listing hazardous waste as F999 [R315-50-9(1)].

MD was an incapacitating or lethal toxic irritant and vesicant agent investigated toward the end of World War I, but it was never employed. DSHW suggested including MD specifically in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including MD specifically as a listed hazardous waste rests on two points:

- 1. There is no reason to believe that MD ever existed in Utah other than, perhaps, in small laboratory samples; and
- 2. MD has not been stockpiled or used as a munitions fill in the United States and was not included in any CAIS.

Note also that arsenic-containing waste not specifically listed as hazardous waste may be classified as hazardous waste under the EPA toxicity characteristic (incorporated under DSHW regulation R315-2-9) as D004 if it leaches arsenic at levels greater than or equal to 5 mg/L.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

5. DF (Methylphosphonyl Difluoride) CAS Reg. No. 676-99-3

$$CH_3P(=0)F_2$$

A. Background

DF is a component of G agent binary munitions. A binary munition generally consists of two liquids that are not very toxic until they are mixed together. The mixing is intended to occur after the munition is armed and on the way to its

military target. For example, the two binary components DF and isopropyl alcohol would react to form sarin (GB). To prevent accidental or malicious formation of a binary mixture, only one member of a binary pair is stored at any one installation. Although some DF may be maintained in the Defense Department binary chemical stockpile, none is located in Utah, and DF is not included in any CAIS.

B. Physicochemical Properties

DF hydrolyzes in water almost instantaneously. Other environmentally relevant information on DF is presented in Table 7.

C. Toxicity

Table 8 shows some intravenous LD_{50} values for DF in different mammalian species. It may be concluded that DF is about three orders of magnitude less toxic than the G agents.

D. Discussion

DF is not currently regulated by EPA under the RCRA program and is not currently incorporated into DSHW regulations. Thus, DF is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. DF content is not used as a basis for listing hazardous waste as F999 [R315-50-9(1)].

DF is a relatively nonhazardous component of G agent binary munitions. DSHW suggested including DF in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

TABLE 7 Environmentally Relevant Properties of DF

Property	Data	Reference
Empirical formula	CH₃F₂PO	NA
Molecular weight (MW), g/mol	100.1	NA
Density, g/mL	1.359/25°C	HQ/DA,DN,AF 1990
	1.3609/25°C	Beilstein Sys. No. 405
Melting point, °C	-37.1	HQ/DA,DN,AF 1990
Boiling point, °C	98-99	Beilstein Sys. No. 405
	22/27 torr	Beilstein Sys. No. 405
Vapor pressure at 25°C, torr	36	HQ/DA,DN,AF 1990

The basis for not including DF as a listed hazardous waste rests on three points:

- Although some DF may be maintained in the Defense Department binary chemical stockpile, none is located in Utah, and DF is not included in any CAIS;
- 2. DF, as a component of binary agent munitions, is not acutely toxic, being approximately as toxic as fluoride salts; and
- 3. Were DF to be released to the environment and come in contact with moisture, it would hydrolyze rapidly.

TABLE 8 Comparison of Some Intravenous Acute Toxicities of DF in Different Mammalian Species

Species	LD ₅₀ (mg/kg)
Dog	25.8
Monkey	26.9
Mouse	114
Rat	13.7

Source: Sweet (1987).

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

6. QL [O-Ethyl O-(2-Diisopropylaminoethyl) Methylphosphonite] CAS. Reg. No. 57856-11-8

 $CH_3P(OC_2H_5)(O-CH_2-CH_2-N(CH[CH_3]_2)_2$

A. Background

QL is a component of VX binary munitions. A binary munition generally consists of two liquids that are not very toxic until they are mixed with each other. The mixing is designed to occur after the munition is armed and on the way to its military target. For example, the two binary components QL and a solubilized form of elemental sulfur would react to form VX. To prevent accidental or malicious formation of a binary mixture, only one member of a binary pair is stored at any one installation. Although some QL may be maintained in the Defense Department binary chemical stockpile, none is located in Utah and QL is not included in any CAIS.

B. Physicochemical Properties

QL, a liquid, is unstable in air. It will ignite without application of spark or flame at 129°C. When QL encounters moisture, it hydrolyzes very rapidly (HQ/DA,DN,AF 1990). Other environmentally relevant information on QL is presented in Table 9.

TABLE 9 Environmentally Relevant Properties of QL

Property	Data	Reference
Empirical formula	C ₁₁ H ₂₆ NO ₂ P	NA
Molecular weight (MW), g/mol	235	NA
Density, g/mL	0.908/25°C	HQ/DA,DN,AF 1990
Boiling point, °C	232	HQ/DA,DN,AF 1990
Vapor pressure at 25°C, torr	0.01	HQ/DA,DN,AF 1990

C. Toxicity

The intravenous LD_{50} s of QL are 204 mg/kg in mice and 164 to 208 mg/kg in rabbits (HQ/DA,DN,AF 1990). It may be concluded that QL is about three orders of magnitude less toxic than the G agents.

D. Discussion

QL is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, QL is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. QL content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

QL is a relatively nontoxic component of VX binary munitions. DSHW suggested including QL in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including QL as a listed hazardous waste rests on three points:

- Although some QL may be maintained in the Defense
 Department binary chemical stockpile, none is located in Utah,
 and QL is not included in any CAIS;
- 2. QL, as a component of binary agent munitions, is not acutely toxic, being approximately as toxic as fluoride salts; and
- 3. Were QL to be released to the environment and come in contact with moisture, it would hydrolyze rapidly.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

7. Chlorosarin (Chloro-GB or O-Isopropyl Methylphosphonochloridate) CAS Reg. No. 1445-76-7

 $CH_3-P(=O)(O-CH[CH_3]_2)CI$

A. Background

Chlorosarin was an intermediate used in the "salt" process for manufacturing GB (sarin) (Nemeth 1989). There is no reason, however, to believe that chlorosarin would be present in plant-run GB. Thus, it is doubtful that chlorosarin, which undergoes very facile hydrolysis, would ever have been found in GB munitions or formulations. As an intermediate, chlorosarin has only an extremely slight potential of being found at GB manufacturing sites. Chlorosarin is not now and never was a chemical agent. Hence, it was never loaded into munitions in the United States or included in any CAIS.

B. Physicochemical Properties

Larsson (1958) reported that chlorosarin hydrolyzes at pH 7 and 25°C at a rate about 5,000 times as great as that of GB (i.e., fluorosarin). On the basis of those results, the half-life would be 46 seconds at pH 7 and 25°C. Other environmentally relevant information on chlorosarin is presented in Table 10.

C. Toxicity

Although the literature contains no information on the acute toxicity of chlorosarin, this compound should be no more toxic than chlorosoman (discussed in Section 8 below), for which the subcutaneous LD₅₀s are 185 mg/kg in the mouse and 153 mg/kg in the rat (Sweet 1987). These values demonstrate toxic levels that are three orders of magnitude higher (i.e., less toxic) than the subcutaneous LD₅₀, 133 μ g/kg, of soman in the mouse (Sweet 1987). This lower toxicity is probably a consequence of chlorosoman's high rate of hydrolysis, a property that chlorosarin would likewise exhibit; chlorosarin is unable to reach the target cholinesterase in nerve synapses before it is hydrolyzed.

D. Discussion

Chlorosarin is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, chlorosarin is not

TABLE 10 Environmentally Relevant Properties of Chlorosarin

Property	Data	Reference
Empirical formula	C₄H₁₀CIO₂P	NA
Molecular weight (MW), g/mol	156.5	NA
Density, g/mL	1.140/25°C	Beilstein Sys. No. 405
Boiling point, °C	51/4 torr	Beilstein Sys. No. 405
	49.1-49.3/2 torr	Beilstein Sys. No. 405
	40/1 torr	Beilstein Sys. No. 405
	36-37/0.5 torr	Beilstein Sys. No. 405
Vapor pressure at 25°C, torr	36	HQ/DA,DN,AF 1990

regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. Chlorosarin content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

Although toxicity data on chlorosarin itself have not been found, tests on a close analogue indicate chlorosarin to be a compound of modest toxicity. DSHW suggested including chlorosarin in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including chlorosarin as a listed hazardous waste rests on four points:

- 1. There is no reason to believe that chlorosarin ever existed (even as a contained intermediate) in any area other than a GB pilot plant or manufacturing plant that used the "salt" process, none of them in Utah;
- Chlorosarin is not now and never was a chemical agent; it was not stockpiled by the Defense Department, it has not been used as a munitions fill, and it is not present in any CAIS;
- 3. Chlorosarin is not acutely toxic, being about three orders of magnitude less toxic than sarin; and
- 4. Should this compound be released to the environment and come in contact with moisture, it would hydrolyze rapidly.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

8. Chlorosoman (Chloro-GD or O-Pinacolyl Methylphosphonochloridate) CAS Reg. No. 1445-76-7

 $CH_3-P(=O)(O-CH[CH_3]C[CH_3)_3)CI$

A. Background

Chlorosoman may have been used as an intermediate in a "salt" process for manufacturing soman (GD) on a pilot scale (see Nemeth 1989 for the method as applied to sarin manufacture). There is no reason, however, to believe that chlorosoman would be present in the soman so prepared. Thus, it is doubtful that chlorosoman, which undergoes very facile hydrolysis, would ever have been found in GD munitions or formulations. As a potential intermediate that may have been used on a pilot scale (but not in Utah), there is a very small potential that chlorosoman may be found at manufacturing sites. Chlorosoman is not now and never was a chemical agent. Hence, it was never loaded into munitions in the United States or included in any CAIS.

B. Physicochemical Properties

By analogy with chlorosarin, chlorosoman should hydrolyze with extreme ease — far more rapidly than soman (i.e., fluorosoman), which itself has at best a short hydrolytic half-life. The empirical formula for chlorosoman is $C_7H_{16}CIO_2P$; the molecular weight is 198.6.

C. Toxicity

The subcutaneous LD_{50} s for chlorosoman are 185 mg/kg in the mouse and 153 mg/kg in the rat (Sweet 1987). These values demonstrate toxic levels that are three orders of magnitude greater (i.e., less toxic) than the subcutaneous LD_{50} , 133 μ g/kg, of soman in the mouse (Sweet 1987). This lower toxicity is probably a consequence of chlorosoman's high rate of hydrolysis; it is unable to reach the target cholinesterase in nerve synapses before it is hydrolyzed.

D. Discussion

Chlorosoman is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, chlorosoman is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)].

Neither is chlorosoman content recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

Chlorosoman is a compound of modest toxicity. DSHW suggested including chlorosoman in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including chlorosoman as a listed hazardous waste rests on five points:

- 1. Chlorosoman, according to available information, could never have existed except as an intermediate at certain soman pilot plant facilities, none of them in Utah;
- 2. Only small amounts of soman, and, hence, possibly chlorosoman, were ever made;
- 3. Chlorosoman is not now and never was a chemical agent; it was not stockpiled by the Defense Department, it has not been used as a munitions fill, and it is not present in any CAIS;
- 4. Chlorosoman is not extremely acutely toxic, being about three orders of magnitude less toxic than soman; and
- 5. Should this compound be released to the environment and come in contact with moisture, it would hydrolyze rapidly.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

9. CX (Phosgene Oxime) CAS Reg. No. 1794-86-1

 $Cl_2C = NOH$

A. Background

CX, an extremely painful irritant "nettle gas," undergoes thermal decomposition near its boiling point. It is extremely (even explosively) unstable in the presence of metals or other impurities, and even when pure it is stable only for one or two months (HQ/DA,DN,AF 1990). Furthermore, CX in glass vessels is stabilized by certain solvents (HQ/DA,DN,AF 1990). CX persists in soil for about

2 hours (HQ/DA,DN,AF 1990). It was never more than a laboratory-scale chemical agent, is not in the U.S. military stockpile, and was not included in any CAIS.

B. Physicochemical Properties

CX hydrolyzes slowly in neutral water and reacts violently in basic solutions (HQ/DA,DN,AF 1990). According to Penski (1993), the Antoine equation for this substance as the liquid (supercooled below the melting point) is:

$$log P (torr) = 9.5243146 - 2838.40258/(t [°C] + 298.763).$$

For temperatures below the melting point, the vapor pressure for the solid would be obtained by using a suitable correction to the estimate for the supercooled liquid. Environmentally relevant properties of CX are given in Table 11.

C. Toxicity

Urticants, the class of chemicals to which phosgene oxime belongs, are compounds of disagreeable penetrating odor that cause immediate severe burning sensations, intense pain, and numbness. Phosgene oxime is one of the most violently irritating substances known. It produces immediate feelings varying from a mild prickling to almost intolerable pain, leading to its description as a "nettle gas." The vapors are extremely irritating to the eyes. Very low concentrations can cause inflammation, tearing, and temporary blindness; higher concentrations may cause corneal corrosion and dimming of vision. When CX comes in contact with the skin, the area becomes pale in 30 seconds and a red ring surrounds it. Subcutaneous edema follows in about 15 minutes and a wheal forms. The

TABLE 11 Environmentally Relevant Properties of CX

Property	Data	Reference
Empirical formula	CHCLNO	NA
Empirical formula	CHCl₂NO	
Molecular weight (MW), g/mol	113.94	NA
Density, g/mL	1.970 (estimate)	
Melting point, °C	39	Penski 1993
Boiling point, °C	128.5 ± 8.8	Penski 1993
Vapor pressure at 25°C, torr	4.16	Estimate from log P (see text)
Log K _{ow}	-0.53	Estimate from log P (see text)
Aqueous solubility, g/L	700 as the hydrate	Edgewood Arsenal 1974

blanched area turns brown and necrotic in about 24 hours, and a scab forms in about a week. The scab usually falls off in three weeks. The site may itch throughout healing, which in some cases takes more than two months (Edgewood Arsenal 1974; HQ/DA,DN,AF 1990).

The human inhalation LCt₅₀ (concentration x time that is lethal to 50% of a population) of phosgene oxime has been estimated at 3,200 mg·min/m³, e.g., 320 mg/m³ for 10 min. The median lowest skin irritant concentration in air for a 10-second vapor exposure was estimated at 1 mg·min/m³; the effects of the agent became unbearable after 1 minute at 3 mg/m³ (HQ/DA,DN,AF 1990). The minimum amount (dissolved in benzene) required to damage 1 cm² of skin was 200 µg (Edgewood Arsenal 1974).

D. Discussion

CX is not currently regulated under the RCRA program by EPA. However, CX is currently regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. CX content is also currently designated as a basis for listing hazardous waste as F999 [R315-50-9(1)].

CX is an extreme irritant but is not stable or persistent. The basis for not including CX as a listed hazardous waste rests on four points:

- 1. Only small amounts of CX were ever made;
- 2. As far as is known, CX has only been used in minuscule quantities (for research purposes) in Utah;
- It was never more than a laboratory-scale chemical agent, is not in the U.S. military stockpile and was not included in any CAIS; and
- 4. CX is extremely unstable.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW proposes the following:

- Remove current 40 CFR 261.33(e) P999 designation in R315-2-11(e).
- Remove current 40 CFR 261.31 F999 designation in R315-2-10(e).

 Remove from 40 CFR 261 Appendix VII basis for listing hazardous waste F999 in R315-50-9(1).

10. DP (Diphosgene or Trichloromethyl Chloroformate) CAS Reg. No. 503-38-8

 $CI-C(=0)-O-CCI_3$

A. Background

DP is a dimer of phosgene (CG). It has a much higher boiling point and lower vapor pressure than CG. DP was first used by the Germans at the battle of Verdun in May 1916; close to the battlefront, the Germans found it easier to load shells with DP than with CG (Prentiss 1937). It was subsequently used by the British (Waitt 1944). DP is not part of the present U.S. chemical stockpile and is not present in any CAIS.

B. Physicochemical Properties

DP hydrolyzes slowly at ambient temperatures. DP is unstable in storage by virtue of its reversion to CG; metals catalyze this reaction (HQ/DA,DN,AF 1990). Table 12 lists environmentally relevant properties for DP. Note that the vapor pressure at 20°C (Table 12) is about one-fourth that of water (Weast 1980), indicating that DP should not persist long in the environment.

TABLE 12 Environmentally Relevant Properties of DP

Property	Data
	
Empirical formula	C ₂ Cl ₄ O ₂
Molecular weight (MW), g/mol	197.85
Density, g/mL	1.653/20°C
Melting point, °C	-57
Boiling point, °C	127-128
Vapor pressure at 20°C, torr	4.2 (1/0°C)
Aqueous solubility, g/L	Limited

Source: HQ/DA,DN,AF (1990).

C. Toxicity

DP can produce delayed or immediate casualties, depending on the dosage received. Because the body converts DP to CG, the systemic effects are the same for both agents. Immediate symptoms may follow exposure to a high concentration of DP; a delay of 3 hours or more may elapse before exposure to a low concentration causes ill effects. DP's effects are cumulative (HQ/DA,DN,AF 1990). The inhalation LC_{50} in the mouse is 3,600 mg/m³/10 min (Sweet 1987). The military estimates an LCt_{50} of 3,000 mg-min/m³ for resting troops (HQ/DA,DN,AF 1990). No multiple-dose data are available for DP.

D. Discussion

DP is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, DP is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. DP content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

DP is an incapacitating or lethal choking agent that was of some interest to the military. DSHW suggested including DP in a draft rule it released to the Army for review in February 1996. Hence, it is evaluated herein.

The basis for not including DP as a listed hazardous waste rests on four points:

- 1. There is no reason to believe that DP ever existed in any U.S. area other than a World War I laboratory, pilot plant, or test facility, certainly not in Utah;
- 2. DP is not stockpiled by the Defense Department, it has not been used as a munitions fill, and it is not included in any CAIS;
- 3. DP is too unstable to have survived in munitions or other containers over the long period since it would reasonably have been made and packaged. Had some vessel or munition containing this agent survived, the agent itself would have reverted to the monomer, CG; and
- 4. Should DP be released to the environment and come in contact with moisture, it would volatilize or it would hydrolyze rapidly.

In accordance with the criteria defined in Section VII.A of the Preamble, DSHW does not propose addition of this chemical to its regulations in any capacity.

11. PS (Chloropicrin) CAS Reg. No. 76-06-2

Cl₃C-NO₂

A. Background

The military use of PS, a volatile material, as a powerful lacrimator (tear-producing agent, tear gas) was begun by the Russians in August 1916 (Prentiss 1937). All the warring countries employed PS during World War I — either alone or mixed with other materials. It was stockpiled, but not used, during World War II. It is not authorized for the U.S. military (HQ/DA,DN,AF 1990). PS also has been used as a pesticide and soil sterilant (Beilstein Sys. No. 6). PS is not part of the U.S. chemical stockpile, but it was included in some CAIS.

B. Physicochemical Properties

The vapor pressure of PS at any temperature t (°C) may be calculated from the following equation (Sartori 1943):

$$\log p \text{ (torr)} = 8.2424 - 2045.2/(273 + t).$$

PS is not subject to hydrolysis; it does decompose under the influence of light (HQ/DA,DN,AF 1990). PS persists approximately 6 hours in vegetated fields (HQ/DA,DN,AF 1990). Environmentally relevant properties of PS are given in Table 13.

C. Toxicity

Table 14 shows some acute toxicities of PS in different mammalian species by different routes of administration. PS is a powerful irritant whose vapors cause nose and throat irritation, coughing, nausea, and vomiting. As an eye irritant, it produces immediate burning, pain, and tearing. Even in very limited concentrations, PS causes the eyelids to close. In high concentrations, PS damages the lungs, causing pulmonary edema. In liquid form it can cause severe burns on the skin that generally result in blisters and lesions. The lowest irritant concentration is 9 mg-min/m³. The LCt₅₀ (presumably an estimate for humans) is 2,000 mg-min/m³ (HQ/DA,DN,AF 1990).

D. Discussion

PS is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, PS is not regulated under the

TABLE 13 Environmentally Relevant Properties of PS

Property	Data	Reference
Empirical formula	CCI₃NO₂	NA
Molecular weight (MW), g/mol	164.38	
Density, g/mL	1.6483/25°C	Beilstein Sys. No. 6
Melting point, °C	-69	HQ/DA,DN,AF 1990
Boiling point, °C	112	Beilstein Sys. No. 6
Vapor pressure, torr	23.81/25°C	Sartori 1943
Aqueous solubility, g/L	1.621/25°C	Beilstein Sys. No. 6
K _H , atm·m³/mol	3.2 x 10 ⁻³ (estimate)	Estimate from log P (see text)
Log K _{oc}	1.806 (estimate)	Estimate from log P (see text)

TABLE 14 Comparison of Some Acute Toxicities of PS by Different Routes of Administration in Rodent Species

Route	Type of Exposure	Species	Toxicity
Intravenous	LD ₅₀	Guinea pig	4,200 µg/kg
Oral	LD ₅₀	Rat	250,000 μg/kg
Inhalation	LC ₅₀	Mouse	1,600 mg/m³/10 min
Intraperitoneal	LD ₅₀	Mouse	25,000 μg/kg

Source: Sweet (1987).

State of Utah P999 hazardous waste code [R315-2-11(e)]. Its content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

PS is extremely irritant and presumably stable in munitions, but it is too volatile to be persistent. The Army suggested evaluating PS because it was used as a chemical incapacitating agent (not as a lethal agent) during Word War I. Hence, it is evaluated herein. PS was used extensively in World War I and stockpiled in World War II, but it is not now in the U.S. military stockpile. PS is included in some CAIS.

The basis for not including PS as a listed hazardous waste rests on two points:

- 1. PS is not stockpiled by the Defense Department, and it is not in use as a munitions fill; and
- 2. Should PS be released to the environment, it would volatilize rapidly.

Although PS is included in some CAIS, as indicated in Section VII.A of the Preamble, DSHW does not propose regulating riot control agents, such as tear gas. In accordance with the criteria defined in Section VII.A, DSHW does not propose addition of this chemical to its regulations in any capacity.

12. CN (Chloroacetophenone) CAS Reg. No. 532-27-4

$$C_6H_5-C(=0)-CH_2CI$$

A. Background

CN is a lacrimator developed after World War I that was formerly used as a riot-control agent; it is considered obsolete for military employment (HQ/DA,DN,AF 1990). CN is the active ingredient of the personal protection agent "Mace" and hence is a commercial chemical used by private industry. CN is not part of the U.S. chemical stockpile, but was included in some CAIS.

B. Physicochemical Properties

The hydrolysis of CN, even in boiling water, is extremely slow (Franke 1967). Vapor pressures have been reported for various temperatures:

t (°C)	P (torr)	Reference
0	0.0026	HQ/DA,DN,AF 1990
10	0.00107	Beilstein Sys. No. 639
20	0.0041	HQ/DA,DN,AF 1990
50	0.128	Beilstein Sys. No. 639
51.7	0.152	HQ/DA,DN,AF 1990
102	5	Beilstein Sys. No. 639
120	10	Beilstein Sys. No. 639

Data from 10 to 51.7° C, expressed as In P and 1/T, form a very linear set, for which the equation is In P (torr) = 31.6164 - 10.877.3/T (K). Other environmentally relevant data for CN are summarized in Table 15.

C. Toxicity

Table 16 shows some acute toxicities of CN in different mammalian species by different routes of administration. CN is a moderately toxic tear-producing irritant (Panel on Cholinesterase Reactivator Chemicals et al. 1984). The estimated human LCt₅₀ is 7,000 mg·min/m³ when the compound is dispersed from solvent, e.g., 100 mg/m³ for 70 min. The human ICt₅₀ (concentration x time that is incapacitating to 50% of a population) is 80 mg·min/m³ (HQ/DA,DN,AF 1990).

CN quickly irritates the eyes and upper respiratory passages. In higher concentrations it causes copious tearing, a tingling sensation, burning and pain of the nose and throat, and burning and itching on tender areas of the skin, especially areas wet by perspiration. High concentrations can cause blisters. The effects are similar to those of sunburn, are "entirely harmless," and disappear in a few hours. Some people experience nausea after exposure to CN (HQ/DA,DN,AF 1990). Animals that died from oral administration of CN showed congestion of the lungs, stomach and intestine, and congestion and hemorrhages of the thymus. Kidney and liver necrosis was seen in many animals. Gross contamination of the eyes with CN can cause severe and permanent corneal injury. CN is a strong skinsensitizing agent, but rarely acutely toxic (Panel on Cholinesterase Reactivator Chemicals et al. 1984).

Results of National Toxicology Program carcinogenicity inhalation testing of this compound were equivocal in rats and negative in mice (National Institute for Occupational Safety and Health [NIOSH] 1993).

D. Discussion

CN is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. Thus, CN is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], nor is its content recorded as a basis for listing hazardous waste as F999 [R315-50-9(1)].

CN is an effective lacrimator (tear gas) of moderate lethality. It is presumably stable in munitions or the environment. It is sufficiently temporary in its effects that it is carried as a defense against muggers. The Army suggested evaluating CN because it has been used as a riot control agent by civilian entities (not as a lethal agent). Hence, it is evaluated herein.

TABLE 15 Environmentally Relevant Properties of CN

Property	Data	Reference
Empirical formula	C ₈ H ₇ CIO	NA
Molecular weight (MW), g/mol	154.59	NA
Density, g/mL	1.318/20°C (solid)	HQ/DA,DN,AF 1990
	1.187/58°C (liquid)	HQ/DA,DN,AF 1990
Melting point, °C	56.5	Beilstein Sys. No. 639
Boiling point, °C	248	HQ/DA,DN,AF 1990
Vapor pressure, torr	0.00756 (solid, 25°C)	By linear regression (see text)
Log K _{ow}	1.34	Estimate
Aqueous solubility, g/L	1.0	Franke 1967
K _H , atm·m³/mol	1.5 x 10 ⁻⁶ /25°C	Estimate from log P (see text)
Log K _{oc}	1.43	Estimate from log P (see text)

TABLE 16 Comparison of Some Acute Toxicities of CN by Different Routes of Administration in Rodent Species

Route	Species	LD ₅₀ (mg/kg)
Intravenous	Mouse	81
Intravenous	Rat	41
Intravenous	Rabbit	30
Orai	Mouse	139
Oral	Rat	50
Oral	Rabbit	118
Oral	Guinea pig	158
Intraperitoneal	Mouse	60
Intraperitoneal	Rat	36
Intraperitoneal	Guinea pig	17

Source: Sweet (1987).

The basis for not including CN as a listed hazardous waste rests on two points:

- CN is a virtually unrestricted article of commerce, widely kept (as "Mace") for self-protection, such that its regulation would affect many non-governmental users; and
- 2. CN is not stockpiled by the Defense Department as a chemical agent.

Although CN is included in some CAIS, as indicated in Section VII.A of the Preamble, DSHW does not propose regulating riot control agent, such as tear gas. In accordance with the criteria defined in Section VII.A, DSHW does not propose addition of this chemical to its regulations in any capacity.

13. DICDI (N,N'-Diisopropyl Carbodiimide) CAS Reg No. 693-13-0

C7H14N2

A. Background

DICDI is an additive used to remove moisture that might form in or diffuse into G or V agents during storage. No more than about 1.5% DICDI in GB is required by military specifications (Rosenblatt et al. 1996).

B. Physicochemical Properties

The half-life of DICDI in water at 25°C and pH 7 is estimated as 31.6 hours; at pH 9.4, the half-life is calculated as 3,600 hours (Williams and Ibrahim 1981).

C. Toxicity

DICDI's intravenous LD_{50} in mice is 56 mg/kg (compared with 0.113 mg/kg for GB) (Sweet 1987), making DICDI about 500 times less intravenously toxic than GB in mice.

D. Discussion

DICDI is not currently regulated under the RCRA program by EPA and, hence, is not currently incorporated into DSHW regulations. DICDI is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], and DICDI

content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

DICDI is not an agent, but rather an additive. Hence, it should not be considered for listing as a "P" commercial chemical product. An additional consideration is whether the chemical should be listed as a hazardous waste constituent [R315-50-10]. The available data indicate that DICDI is a relatively nontoxic compound, being some two orders of magnitude less toxic than the nerve agent that it is used to stabilize. In addition, the only toxicity information available is intravenous, which has little relation to effects of this chemical on human health and the environment. Also, the chemical is only a very minor component of stabilized nerve agent. Finally, the nerve agent itself is the primary concern. DSHW is therefore not proposing to include this chemical in the proposed rule in any capacity.

14. MA (Methylphosphonofluoridic Acid) No CAS Number Found

CH₄FO₂P

A. Background

MA is not known to be present in any chemical munition. MA is known to form almost instantaneously when DF (methylphosphonyl difluoride, a binary GB component) comes in contact with water (HQ/DA,DN,AF 1990). DF is discussed in Section 5.

B. Physicochemical Properties

Half-lives (presumably at 25°C) for hydrolysis of MA are 162 days at pH 7, 90 days at pH 4, and 47 days at pH 3 (HQ/DA,DN,AF 1990).

C. Toxicity

MA has an oral LD_{50} of 300 mg/kg in the rat (Sweet 1987).

D. Discussion

MA is not currently regulated under the RCRA program by EPA and, hence, is not currently incorporated into DSHW regulations. MA is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. MA content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

The source of MA, DF, is a relatively nonhazardous component of G agent binary munitions. Although the proximate source of MA (i.e., DF) is maintained in the Defense Department binary chemical stockpile, none is located in Utah. DF is not proposed for listing in any capacity. Hence, DSHW does not propose MA for listing in any capacity.

15. TBA (Tributylamine)

CAS Reg. No. 102-82-9

 $C_{12}H_{27}N$

A. Background

TBA is a stabilizer for weapons-grade GB, added in small amounts (not over about 5%) to neutralize acid formed by undesirable hydrolysis of the GB (see Rosenblatt et al. 1996).

B. Physicochemical Properties

TBA, a liquid boiling at 213°C, is not subject to hydrolysis, although it is oxidized by bleach, a common agent decontaminant (Rosenblatt et al. 1996; Rosenblatt and Burrows 1982).

C. Toxicity

The oral LD₅₀ of TBA in the rat is 540 mg/kg (Sweet 1987).

D. Discussion

TBA is not currently regulated under the RCRA program by EPA and hence is not currently incorporated into DSHW regulations. TBA is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], and TBA content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

TBA is not an agent, but rather an additive. Hence, it should not be considered for listing as a "P" commercial chemical product. An additional consideration is whether the chemical should be listed as a hazardous waste constituent [R315-50-14]. The available data indicate that TBA is a relatively nontoxic compound, being some three orders of magnitude less toxic than the nerve agent that it is used to stabilize. Also, the chemical is only a very minor component of stabilized nerve agent. Finally, the nerve agent itself is the primary

concern. DSHW is therefore not proposing to include this chemical in the proposed rule in any capacity.

16. DIMP (Diisopropyl Methylphosphonate) CAS. Reg. No. 1445-75-6

 $CH_3P(=O)(OCH[CH_3]_2)_2$

A. Background

DIMP is an intermediate in one method of producing GB, as well as a potential impurity of GB. It has been found in groundwater at the Rocky Mountain Arsenal (RMA), Colorado (as a byproduct of the GB manufacturing formerly conducted there), and it has persisted there for many years. DIMP has been commercially available in the open market (Strum 1997).

B. Physicochemical Properties

DIMP is a colorless liquid. Its reported empirical vapor pressure equation (Rosenblatt et al. 1975) is:

$$log P (torr) = 9.8571 - 3105/T(K)$$
.

This equation gives a vapor pressure of 0.28 torr at 25°C, compared with a vapor pressure of 1.49 torr estimated by the method of Fishtine as presented by Lyman et al. (1990).

The estimated hydrolysis half-life of DIMP in water at 10°C was 687 years (Rosenblatt et al. 1975); the half-life in soil was estimated as 2 years (Spanggord et al. 1979). In contact with RMA sandy loam at room temperature, aqueous DIMP showed no hydrolysis; under comparable conditions, Lakewood sand catalyzed hydrolysis with a half-life of about 300 hours (Kingery and Allen 1994). Thus, it appears that some soils catalyze DIMP decomposition while others do not.

Table 17 presents environmentally relevant properties of DIMP. Because of its comparative stability towards hydrolysis, DIMP, if released to the environment, would have a significant potential to migrate into groundwater.

TABLE 17 Environmentally Relevant Properties of DIMP

Property	Data	Reference
For disast formula	CHOR	NIA
Empirical formula	$C_7H_{17}O_3P$	NA
Molecular weight (MW), g/mol	180.18	NA
Density, g/mL	0.976/25°C	Rosenblatt et al. 1975
Boiling point, °C	174	Rosenblatt et al. 1975
Vapor pressure at 25°C, torr	0.28	Estimate from log P (see text)
Log K _{ow}	1.35	Major 1989
Aqueous Solubility, g/L	Infinitely miscible	Major 1990
K _н , atm·m³/mol	2.71 x 10 ⁻⁷ /25°C	Estimate from log P (see text)
Log K _{oc}	1.44	Estimate from log P (see text)

C. Toxicity

There is no evidence that DIMP is particularly toxic to man. Acute oral LD_{50} values in several species ranged from 503 mg/kg in female mink to 1,490 mg/kg in mallard ducks. In the mink, clinical signs of acute intoxication included salivation, lethargy, weakness, vomiting, and immobilization (Roberts and Hartley 1992). Table 18 shows the median lethal doses of DIMP in other experimental animals by oral administration.

Dacre and Rosenblatt (1987) cited 96-hour DIMP aquatic organism toxicity studies by Bentley et al. (1976) without giving actual findings, except to say that there was essentially no bioconcentration in bluegills.

On the basis of a no-observed-adverse-effect level at the highest administered dose of DIMP in a 90-day study in dogs, and an uncertainty factor of 1,000, EPA determined a reference dose (RfD) of 80 μ g/kg/day, a drinking water

equivalent level (DWEL) of 2.8 mg/L, and a lifetime drinking water health advisory value of 600 µg/L. Because of a lack of information, the compound was assigned by EPA to group D (not classified as to human carcinogenicity) (Roberts and Hartley 1992).

TABLE 18 Oral Toxicity of DIMP in Three Mammalian Species

D. Discussion

DIMP is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. DIMP is not currently regulated under the State of Utah P999 hazardous waste code

Species	LD ₅₀ (mg/kg)	
Cattle	750	
Mouse	1,041	
Rat	826	

Source: Sweet (1987).

[R315-2-11(e)]. DIMP content is not treated as a basis for listing hazardous waste F999 [R315-50-9]. However, DIMP is being addressed pursuant to the Dugway Proving Ground (Utah) installation restoration program, as well as the installation restoration program at the RMA.

DIMP is not an agent, but rather a potential impurity of GB. Hence, it should not be considered for listing as a "P" commercial chemical product. An additional consideration is whether the chemical should be listed as a hazardous waste constituent [R315-50-14]. The available data indicates that DIMP is a relatively nontoxic compound, being some three to four orders of magnitude less toxic than GB. Also, the chemical is only a potential impurity. While DIMP is also an intermediate in the manufacture of GB, because GB was not manufactured in Utah, DIMP from manufacturing would not be expected to be found in Utah. Finally, the nerve agent itself is the primary concern with process wastes. DSHW is therefore not proposing to include this chemical as a hazardous waste constituent.

DIMP could also be considered as a groundwater monitoring constituent, being a good indicator for the presence of release of GB from land disposal units. However, there are several additional compounds that are far better indicators of the presence of releases of GB, such as IMPA, the principal hydrolysis product of GB (Rosenblatt et al. 1996). DSHW therefore does not propose addition of DIMP to the proposed rule regulations in any capacity.

17. IPA (Isopropyl Alcohol or 2-Propanol) CAS Reg. No. 67-63-0

C₃H₈O

A. Background

IPA is a binary GB component (along with DF, discussed above), as well as the product of the extremely slow hydrolysis of DIMP and methylphosphonic acid. Far more important, it is sold commercially as "rubbing alcohol" for a variety of domestic uses.

B. Physicochemical Properties

IPA is completely miscible with water and is stable in water over a wide pH range. IPA melts at -89.5°C, boils at 82.4°C, and has a specific gravity of 0.78 (Weast 1980). With its low boiling point, pure IPA is rather flammable, with a flash point of 53°F (Lewis 1991).

C. Toxicity

IPA is generally regarded as virtually harmless, though not recommended for ingestion. The oral rat LD_{50} is 5,045 mg/kg (compared with 7,060 mg/kg for ethanol) (Sweet 1987).

D. Discussion

IPA is not currently regulated under the RCRA program by EPA, and is not currently incorporated into DSHW regulations. IPA is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], nor is IPA content recorded as a basis for listing hazardous waste as F999 [R315-50-9].

IPA is a relatively nonhazardous component of G agent binary munitions. It is also a very commonly used household product with a very low toxicity. Hence, it should not be considered for listing as a "P" commercial chemical product. An additional consideration is whether the chemical should be listed as a hazardous waste constituent [R315-50-14]. IPA is a relatively nontoxic compound. In addition, although some IPA may be maintained in the Defense Department binary chemical stockpile, none is located in Utah, and IPA is not included in any CAIS.

In accordance with the criteria defined in the Preamble, Section VII.A, DSHW does not propose addition of this chemical to its regulations in any capacity.

18. DMDS (Dimethyl Disulfide) CAS Reg. No. 624-92-0

CH₃-S-S-CH₃

A. Background

Like DIMP, DMDS has been associated with RMA. There are at least two possible sources of DMDS: (1) methanethiol, which is easily air-oxidized to DMDS, might have been used by Shell Chemical Co. at RMA as a precursor; or (2) DMDS could have been used as a sulfur carrier in binary VX munitions. No stockpiles of VX binary munitions are located in Utah, and VX was not manufactured in Utah. Therefore, the amounts brought into Utah would at most have been be quite small (e.g., for research purposes). There is no evidence that DMDS attributable to the military was ever found in Utah.

B. Physicochemical Properties

DMDS melts at -64°C and boils at 109.7°C (Weast 1980).

C. Toxicity

DMDS has an LD₅₀ (route unspecified) of 138 mg/kg (Sweet 1987).

D. Discussion

DMDS is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. DMDS is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)], and DMDS content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

DMDS is not an agent, but rather may have been used in the manufacturing process for VX binary munitions. Such munitions were not produced in Utah, and stockpiles of VX binary munitions are not stored in Utah. Hence, DMDS should not be considered for listing as a "P" commercial chemical product. An additional consideration is whether the chemical should be listed as a hazardous waste constituent [R315-50-10]. DMDS is not maintained in the Defense Department chemical stockpile in Utah. Military-related DMDS has not been identified in Utah. DMDS is a compound of moderate toxicity. For these reasons, DSHW is not proposing to include this chemical in the proposed rule in any capacity.

19. OXAT (1,4-Oxathiane) CAS Reg. No. 15980-15-1

C₄H₈SO

A. Background

OXAT is a minor — but evidently consistent — product of the hydrolytic decomposition of sulfur mustard (HD) in the presence of excess water, the major product being thiodiglycol (TDG) (Rosenblatt et al. 1996). OXAT is formed and released as HD slowly dissolves in and reacts with water. The presence of OXAT in environmental water samples may be used as an indicator that HD is, or was, in the vicinity.

B. Physicochemical Properties

Environmentally relevant information on OXAT is presented in Table 19.

TABLE 19 Environmentally Relevant Properties of 1,4-Oxathiane

Property	Data	Reference
Empirical formula	C H 80	NA
Empirical formula	C₄H ₈ SO	
Molecular weight (MW), g/mol	104.18	NA
Melting point, °C	-17	Berkowitz et al. 1978
Boiling point, °C	147-150	Berkowitz et al. 1978
Vapor pressure at 25°C, torr	5.3	Berkowitz et al. 1978
Log K _{ow}	0.77	Major 1989
Aqueous solubility, g/L	167 (estimate)	Berkowitz et al. 1978

C. Toxicity

No information is available on the effects of OXAT in humans. Large oral LD₅₀ values are reported for rats, namely 2,830 and 3,000 mg/kg in separate studies (Roberts and Hartley 1992), and for guinea pigs (3,960 mg/kg, ICF KE/Clement 1991). Antemortem observations in the rat studies include coma, ataxia, lacrimation, dyspnea, cyanosis, squinting, paralysis, and hunched posture.

D. Discussion

OXAT is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. OXAT is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. Its content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

1,4-oxathiane should be evaluated because it is a minor — but evidently consistent — product of the hydrolytic decomposition of HD. However, the issue is not toxicity, but its potential usefulness as an indicator of HD environmental contamination, particularly as a groundwater monitoring constituent.

Although OXAT is an easily assayed indicator for the possible presence or former presence of HD in the vicinity, TDG is arguably more suitable for that purpose and is therefore being proposed as a groundwater monitoring constituent for HD in R315-50-14. Listing OXAT in this capacity would be duplicative. DSHW therefore does not propose addition of OXAT to its regulations in any capacity.

20. DITH (1,4-Dithiane) CAS Reg. No. 505-29-3

C₄H₈S₂

A. Background

DITH is a principal product of the thermal decomposition of sulfur mustard (HD), a reaction that also forms 1,2-dichloroethane. This reaction continues at a slow rate over the course of years in any stored specimen of HD (Roberts and Hartley 1992). DITH is released when HD slowly dissolves in water and reacts with it; but there is no evidence of its formation as a result of contact with water. The presence of DITH in environmental water samples may be used as an indicator that HD is, or was, in the vicinity.

B. Physicochemical Properties

DITH is reported (Berkowitz et al. 1978) to have an empirical vapor pressure of:

$$log P (torr) = 7.99 - [2,410/T(K)].$$

Other environmentally relevant information on DITH is presented in Table 20.

C. Toxicity

Vapors of DITH are reported to be irritating to the oral cavity and upper respiratory tract in humans (ICF KE/Clement 1991). The oral LD₅₀ to rats (combined male and female) of 3,473 mg/kg indicates fairly low toxicity. Crusty

TABLE 20 Environmentally Relevant Properties of 1,4-Dithiane

Property	Data	Reference
Empirical formula	C ₄ H ₈ S ₂	NA
Molecular weight (MW), g/mol	120.13	NA
Melting point, °C	111-112	Weast 1980
Boiling point, °C	199-200	Weast 1980
Vapor pressure at 25°C, torr	0.8	Estimate from log P (see text)
Log K₀w	1.85	Major 1989
Aqueous solubility, g/L	11.8 (estimate)	Berkowitz et al. 1978

eyes, nose, or muzzle; hyperactivity; tremors; emaciation; ataxia; and irregular breathing were among the antemortem observations (ICF KE/Clement 1991; Roberts and Hartley 1992).

In a 90-day gavage study in rats, the no observed adverse effects level was 105 mg/kg/day (Roberts and Hartley 1992). On the basis of this result, with an uncertainty factor of 1,000 and a modifying factor of 10, a reference dose (RfD) of 0.01 mg/kg/day was derived (Hartley et al. 1994). Hence, the drinking water equivalent level is 0.4 mg/L, and the lifetime health advisory value is 80 μ g/L (Hartley et al. 1994).

Regression equations relating toxicity for aquatic species to log K_{ow} (1.85) indicated that dithiane is not very toxic to these organisms. The most sensitive species, the saltwater sheepshead minnow, was estimated to have a 96-hour LC₅₀ of 26.5 mg/L (ICF KE/Clement 1991).

D. Discussion

DITH is not currently regulated under the RCRA program by EPA and is not currently incorporated into DSHW regulations. DITH is not regulated under the State of Utah P999 hazardous waste code [R315-2-11(e)]. Its content is not recorded as a basis for listing hazardous waste as F999 [R315-50-9].

DITH should be evaluated because it is a product of the decomposition of HD over time. However, as with OXAT, the concern is not toxicity, but its potential usefulness as an indicator of HD environmental contamination, particularly as a groundwater monitoring constituent.

Although DITH is an easily assayed indicator for the possible presence or former presence of HD in the vicinity, TDG is arguably more suitable for that purpose and is therefore being proposed as a groundwater monitoring constituent for HD in R315-50-14. Listing DITH in this capacity would be duplicative. DSHW therefore does not propose addition of DITH to its regulations in any capacity.

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